

Positron binding to polar molecules

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Before a positron annihilates with an electron in a polyatomic molecule, it usually enters into a quasibound state [1]. A wealth of experimental data on positron-molecule binding are now available. It shows that the binding energy ε_b is strongly enhanced in molecules with large permanent dipole moments [2]. However, there are few calculations of positron binding, and due to the difficulty in treating the electronic states in the presence of a positron, these calculations are not generally considered precise [3].

In this work we study positron-molecule binding theoretically using a simple model. The molecule is modelled as an impenetrable sphere of radius r_0 with a static point dipole \mathbf{D} moment at its centre. Outside the sphere the positron experiences the point dipole's potential:

$$V(\mathbf{r}) = \begin{cases} \infty & \text{if } r \leq r_0, \\ \mathbf{D} \cdot \mathbf{r}/r^3 & \text{if } r > r_0. \end{cases} \quad (1)$$

For this potential the radial Schrödinger equation can be solved analytically in terms of Bessel functions, with the angular part diagonalized numerically. The application of appropriate boundary conditions leads to a simple relationship between ε_b and r_0 , and we consider r_0 as a fitting parameter. Using existing experimental data on binding energies leads to unphysically small values of r_0 for all of the molecules studied. This suggests that electron-positron correlations neglected in (1) play a large role in determining the binding energy. We account for these using the polarization potential $-\alpha/2r^4$ (where α is the molecular dipole polarizability) via perturbation theory; the first-order correction to the binding energy is

$$\Delta\varepsilon_b = \int |\psi(\mathbf{r})|^2 (\alpha/2r^4) d^3\mathbf{r}, \quad (2)$$

where $\psi(\mathbf{r})$ is the ground-state positron wave function. This has enabled accurate predictions of ε_b to be made for a range of organic molecules and hydrogen cyanide, whose binding energy cannot be measured experimentally but has been calculated with the diffusion Monte Carlo (DMC) method [4].

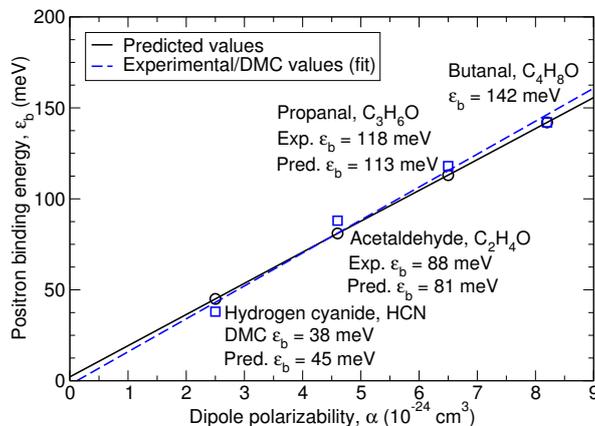


Figure 1: Comparison of predicted ε_b obtained using $D = 2.7$ debye and $r_0 = 0.58$ a.u. for aldehydes and hydrogen cyanide (circles) with experimental values for aldehydes and DMC for HCN (squares).

References

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